Constrained crystals deep convolutional generative adversarial network for the inverse design of crystal structures

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Abstract

Autonomous materials discovery with desired properties is one of the ultimate goals for materials science, and the current studies have been focusing mostly on high-throughput screening based on density functional theory calculations and forward modeling of physical properties using machine learning. Applying the deep learning techniques, we have developed a generative model, which can predict distinct stable crystal structures by optimizing the formation energy in the latent space. It is demonstrated that the optimization of physical properties can be integrated into the generative model as on-top screening or backward propagator, both with their own advantages. Applying the generative models on the binary Bi-Se system reveals that distinct crystal structures can be obtained covering the whole composition range, and the phases on the convex hull can be reproduced after the generated structures are fully relaxed to the equilibrium. The method can be extended to multicomponent systems for multi-objective optimization, which paves the way to achieve the inverse design of materials with optimal properties.